REPORT DOCUMENTATION PAGE	*Form Approved* *OMB No. 0704-0188*

1. REPORT DATE *(DD-MM-YYYY)*	**2. REPORT TYPE**	**3. DATES COVERED** *(From - To)*
July 2015	Technical Paper	July 2015-July 2015

4. TITLE AND SUBTITLE
Boltzmann transport in hybrid PIC HET modeling

5a. CONTRACT NUMBER
In-House

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
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5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER
Q0A5

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Air Force Research Laboratory (AFMC)
AFRL/RQRS
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8. PERFORMING ORGANIZATION REPORT NO.

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Air Force Research Laboratory (AFMC)
AFRL/RQR
5 Pollux Drive
Edwards AFB CA 93524-7048

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
AFRL-RQ-ED-TP-2015-214

12. DISTRIBUTION / AVAILABILITY STATEMENT
Distribution A: Approved for Public Release; Distribution Unlimited.

13. SUPPLEMENTARY NOTES
Technical Paper and Briefing Charts presented at IEPC 2015; Kobe, Japan; 04-10 July 2015. PA#15307.

14. ABSTRACT
Electron transport models are a key source of uncertainty inhibiting first-principal simulation of Hall-effect thruster (HET) physics. Fluid electron models depend heavily on the electron mobility tensor, generally constructed using semi-empirical relationships which require user-adjustable tuning parameters and are based on the assumption of an electron velocity distribution function in local thermal equilibrium. Recently, work in the field of gaseous electronics has produced a variety of self-consistent electron swarm codes, such as the Magboltz code, focused on directly solving the steady Boltzmann trans-port equation including both electromagnetic and collisional processes. In parallel, the community have also developed extensive electron collision databases that include detailed elastic and inelastic collision cross sections for electrons with various gases. In this work, we investigate whether Magboltz can reproduce experimentally observed mobility trends derived from HPHall, a workhorse hybrid-PIC HET simulation code.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**			Justin Koo
Unclassified	**Unclassified**	**Unclassified**	SAR	29	**19b. TELEPHONE NO** *(include area code)* 661-275-5908

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. 239.18

Boltzmann transport in hybrid PIC HET modeling

IEPC-2015-xxx/ISTS-2015-b-xxx

*Presented at Joint Conference of 30th International Symposium on Space Technology and Science, 34th International Electric Propulsion Conference and 6th Nano-satellite Symposium
Hyogo-Kobe, Japan
July 4–10, 2015*

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Abstract: Electron transport models are a key source of uncertainty inhibiting first-principal simulation of Hall-effect thruster (HET) physics. Fluid electron models depend heavily on the electron mobility tensor, generally constructed using semi-empirical relationships which require user-adjustable tuning parameters and are based on the assumption of an electron velocity distribution function in local thermal equilibrium. Recently, work in the field of gaseous electronics has produced a variety of self-consistent electron swarm codes, such as the Magboltz code, focused on directly solving the steady Boltzmann transport equation including both electromagnetic and collisional processes. In parallel, the community have also developed extensive electron collision databases that include detailed elastic and inelastic collision cross sections for electrons with various gases. In this work, we investigate whether Magboltz can reproduce experimentally observed mobility trends derived from HPHall, a workhorse hybrid-PIC HET simulation code.

Nomenclature

E	= magnitude of electric field
E_i	= i^{th} component of electric field
B	= magnitude of magnetic field
B_i	= i^{th} component of magnetic field
T_e	= electron temperature
m_e	= electron mass
n_e	= electron density
j_e	= electron current density
T_n	= neutral temperature
m_n	= neutral mass
k_b	= Boltzmann constant
ν_e	= electron momentum exchange frequency
e	= elementary charge
μ	= scalar electron mobility
ν	= electron momentum exchange collision frequency
Ω_e	= electron Hall parameter

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I. Introduction

HET operation is governed strongly by the rate at which electrons, responding to the applied potential, are able to move towards the anode. While the rate of travel of the electrons is controlled by a number of different physical effects, the strongest driver of electron transport is the imposed magnetic field generated by the magnetic circuit of the device. Experimental measurements and computational simulations have consistently indicated that the electron transport perpendicular to the magnetic field is higher than expected from classical theory. The origin of this so-called anomalous electron mobility (or diffusion) has been attributed to a number of mechanisms including instabilities in the discharge (turbulent fluctuations) and plasma-wall interactions. An additional mechanism which may also contribute to anomalous transport, the deviation of the electron velocity distribution function from local thermal equilibrium, can be simulated by Magboltz,[1] an electron swarm code discussed in more detail in Sec. A. This work focuses on comparison between the electron mobility (including anomalous effects) required by a mainstream hybrid-PIC HET code, HPHall,[2] and the mobility predicted by Magboltz based on the same local fields and plasma conditions experienced in HPHall.

1. Electron mobility in HET simulation

The most widely used computational simulations of HETs, including HPHall, use a hybrid-PIC methodology which relies on a fluid description for the electron fluid. In order to produce realistic results, these codes rely heavily on semi-empirical models for anomalous electron transport which themselves have one or more tuning parameters. These codes are consistently based on a Generalized Ohm's Law description of the electron fluid which reduces (under the assumption of zero convective derivative and the electron velocity being greater than both the neutral and ion velocities) to:

$$\vec{j_e} + \mu \vec{j_e} \times \vec{B} = \mu e n_e \vec{E} + \mu \nabla p \tag{1}$$

where the scalar electron mobility can be written as:

$$\mu = \frac{e}{m_e \nu_e} \tag{2}$$

Expanding Eq. 1 in cartesian coordinates, it is possible to construct a relationship between the accelerating terms and the electron current as follows:

$$\begin{bmatrix} j_x \\ j_y \\ j_z \end{bmatrix} = \frac{1}{1+\mu^2 B^2} \begin{bmatrix} 1+\mu^2 B_x^2 & -\mu B_z + \mu^2 B_x B_y & \mu B_y + \mu^2 B_x B_z \\ \mu B_z + \mu^2 B_x B_y & 1+\mu^2 B_y^2 & -\mu B_x + \mu^2 B_y B_z \\ -\mu B_y + \mu^2 B_x B_z & \mu B_r + \mu^2 B_y B_z & 1+\mu^2 B_z^2 \end{bmatrix} \begin{bmatrix} \mu e n_e E_x + \mu \frac{\partial p}{\partial x} \\ \mu e n_e E_y + \mu \frac{\partial p}{\partial y} \\ \mu e n_e E_z + \mu \frac{\partial p}{\partial z} \end{bmatrix} \tag{3}$$

Assuming that $B = B_z$ (with the z-direction approximating the radial direction) and that all derivatives in the y-direction are zero (approximating azimuthal symmetry), Eq. 3 reduces to a simple one-dimensional form:

$$j_x = \mu_\perp (e n_e E_x + \frac{\partial p}{\partial x}) \tag{4}$$

where

$$\mu_\perp = \frac{\mu}{1+\mu^2 B^2} = \frac{e}{m\nu_e} \frac{1}{1+(\frac{eB}{m\nu_e})^2} = \frac{e}{m\nu_e} \frac{1}{1+\Omega_e^2} \tag{5}$$

Classically, the electron momentum exchange collision frequency is based on interactions between the electrons and other plasma species as follows:

$$\nu_{e,class} = \nu_{e-ion} + \nu_{e-neutral} \tag{6}$$

In practice, to produce realistic HET simulations, it is necessary to dramatically increase the effective electron momentum exchange collision frequency relative to that predicted by purely classical means. This additional collisionality is achieved through the use of both an electron-wall and Bohm collision frequency

in the calculation of the anomalous component of the electron momentum exchange collision frequency as follows:

$$\nu_{e,anom} = \nu_{wall} + \nu_{Bohm} \tag{7}$$

The final form of the effective electron momentum exchange collision frequency is therefore:

$$\nu_e = \nu_{e,class} + \nu_{e,anom} \tag{8}$$

The effect of differing underling models for each of these terms has been studied extensively throughout the literature, but every single model for the anomalous contribution to the collision frequency depends on at least one ad hoc tuning parameters.[a] A consistent feature of the resulting electron mobility profiles which result in good agreement with experimental data is a relatively large anomalous correction which results in a large perpendicular electron mobility in the near-field plume region of the thruster as shown in Fig. 1.

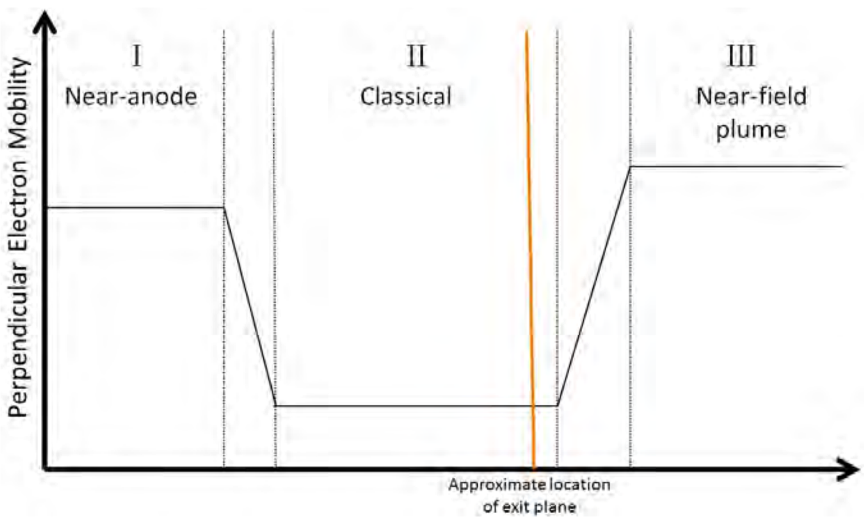


Figure 1: Cartoon schematic of anomalous electron transport regions in typical HET

II. Computational setup

As the stalwart HET simulation code in the EP modeling and simulation community, the use of different mobility models in HPHall has been thoroughly explored in the open literature by many groups including Hofer,[3] Bareilles[4] and Koo.[5] In this paper, we are interested in exploring the ability of Magboltz to provide purely physics-based mobility coefficients to HPHall. In particular, we want to see whether it is possible to get rid of the tuning parameters in a HET code related to electron mobility calculation. While we would prefer to incorporate Magboltz directly into HPHall as a module which explicitly provides the electron mobility, our current HPHall simulations requires mobility evaluation at 1165 node points, with an approximate runtime between one to two minutes per Magboltz calculation. Even if 1165 instances of Magboltz were all run in parallel, this would still dramatically slow HPHall since these coefficients are needed not just at each ion timestep (given that a single timestep in the baseline HPHall takes a few seconds, the code would face a ≈10–100x slowdown), but rather at each electron timestep (which would represent a >1,000x slowdown of the code). Thus, it is clearly prohibitive to couple the two codes in a direct manner. Instead, we use a single snapshot from an HPHall simulation to get input data (fields, densities, etc) for Magboltz. Good agreement between the HPHall mobility and the Magboltz mobility indicates that the non-equilibrium physics of Magboltz are an important component of the anomalous electron transport observed in HETs. A set of HPHall simulations for three operating regimes of a representative sub-kW class HET are used to generate the baseline plasma conditions for this paper (see Table 1).

[a]In fact, a significant factor in the longevity of HPHall is the degree to which the tuning parameters for the Bohm contribution have been successfully calibrated to produce excellent experimental agreement.

Table 1: Performance data from HPHall simulations

HPHall	Thrust (N)	Discharge Voltage (V)	Discharge Current (A)
Mode A	0.0137	250	0.80
Mode B	0.0265	250	1.84
Mode C	0.0141	100	2.00

A. Magboltz

Magboltz[1] is computer simulation program written in FORTRAN for computing electron drifts and diffusion in neutral gas mixtures under the influence of electromagnetic fields. To get the diffusion tensor, a Monte-Carlo integration technique is used to trace mulitple particle trajectories under the influence of both electric and magnetic fields with neutral collisions as described by Fraser.[6] The underlying coordinate frame is based on a cartesian reference where the x-axis is aligned with the electric field and the magnetic field is at a prescribed angle to the electric field in the x-z plane.

The equations of motion for the free flight (between collisions) of an electron in an electromagnetic field are integrated analytically. The free time between collisions is determined by generating a pseudo-random number and then relating it to the collision frequency by the expression:

$$\ln[(1-R)^{-1}] = \int_0^t \nu(t)dt)$$

Neutral gas effects are incorporated in Magboltz through the implementation of both elastic and inelastic collisions including both isotropic and anisotropic angular scattering using the technique of Longo;[7] however, for the simulations presented in this paper, it is assumed that elastic collisions dominate inelastic collisions at all electron energies. This is valid in the case of most noble gases at low energies where inelastic scattering is absent. The collision frequency is determined from an extensive collisional cross section database in Magboltz which includes elastic, inelastic, ionizing and super-elastic collisions along with attachment rates. For Xenon, the gas studied in this paper, the collisional cross sections are shown in Fig. 2.

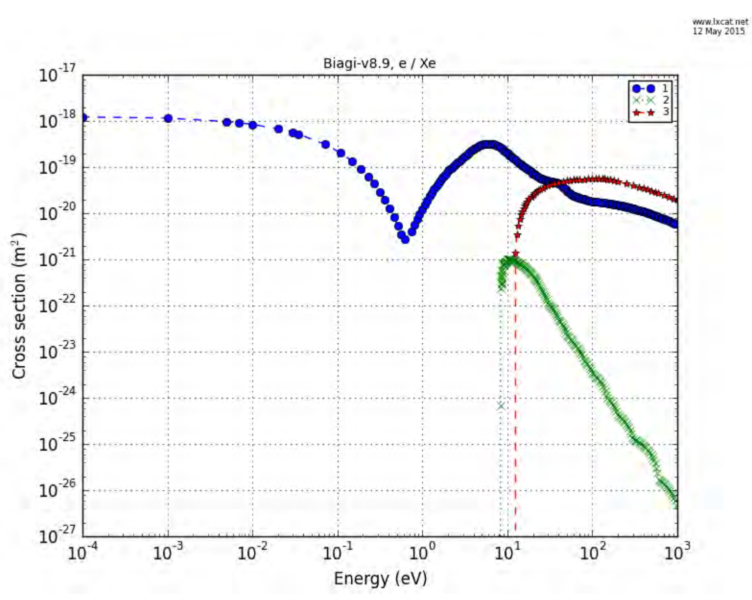


Figure 2: (1) elastic, (2) 1s5 excitation and (3) ionization collision cross section data for Xenon used by Magboltz 10.4 with a mass ratio of $m_e/m_n = 4.2e-6$. Magboltz also has data for 49 additional excitation cross sections not provided above but are used in the simulation. Comprehensive data can be found at `www.lxcat.net`.

From the raw particle trajectories, the diffusion is calculated using the displacement formalism given in

Biagi[1] as:

$$D_{ij} = \frac{1}{2N}\sum[\frac{1}{dt}(q_i - v_i dt)(q_j - v_j dt)] \tag{9}$$

Where the time interval dt is determined by a number of intermittent collisions that reduces the error in the calculation of the diffusion coefficients to be a factor of two of the accuracy of the velocity vectors. The expression is then summed over the number of time intervals. This provides a 2nd order symmetric diffusion tensor which is typically fully populated for cases where the magnetic field is not at a right angle to the electric field. To gather sufficiently smooth statistics, an average of 100,000 particle flights are performed to generate a single diffusion tensor.

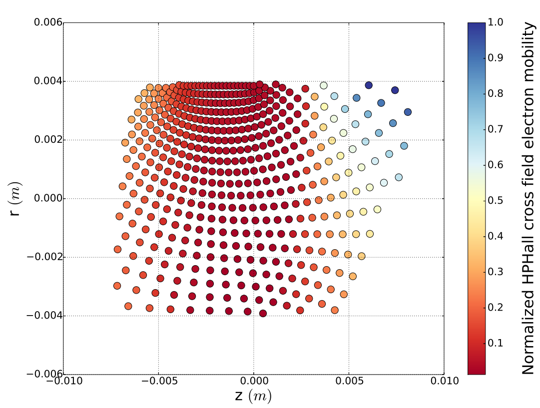
III. Results and Discussion

Using HPHall simulations for a representative sub-kW class HET, the axial and radial electric and magnetic field, neutral particle density and neutral temperature were extracted at each node in the 2d HPHall grid. The magnitude of the total electric and magnetic field is computed along with the angle between the fields at all node points. Using the ideal gas law the neutral pressure is determined from the neutral number density and average neutral temperature. Because the average neutral velocity is significantly smaller than the electron velocity, we approximate the neutrals as stationary. Magboltz then computes the electron diffusion tensor and average electron temperature at each node on the 2d grid. The diffusion tensor is then diagonalized and the Einstein relation $D = \mu_e k_b T/e$ is then applied to convert the principle components of the diffusion tensor to their corresponding mobility counterpart. From the resulting three mobilities, the smallest one is always the perpendicular (cross-field) electron mobility.

A. Mode A: 250V & 0.80A

The perpendicular electron mobility profiles for Mode A as calculated by HPHall and Magboltz are shown in Fig. 3. These data are normalized individually to the highest mobility shown in the field of view. The ratio between the two (HPHall divided by Magboltz) is shown in Fig. 4. Finally, the full dataset for the perpendicular electron mobility as calculated by Magboltz is shown in Fig. 5.

While there is some resemblence between the overall mobility profile calculated by Magboltz in Fig. 5 and the notional mobility profile presented in Fig. 1, it is clear from this data that the Magboltz mobility does not identically reproduce the details of the HPHall mobility. The primary area of concern is the near-anode region, we can hypothesize that the relative error as shown in Fig. 4 is driven by additional inclusion of a electron-wall collision term in HPHall which is clearly not present in the Magboltz simulation. Remarkably, the agreement between Magboltz and the effective perpendicular mobility (as used by HPHall) in the near-field plume region is remarkably good in this case.



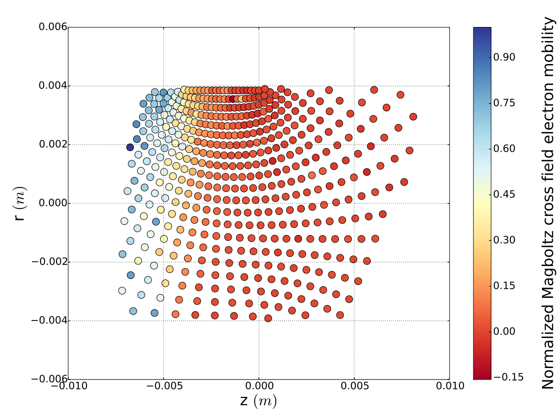


Figure 3: Relative perpendicular electron mobility calculated by HPHall (left) and Magboltz (right)

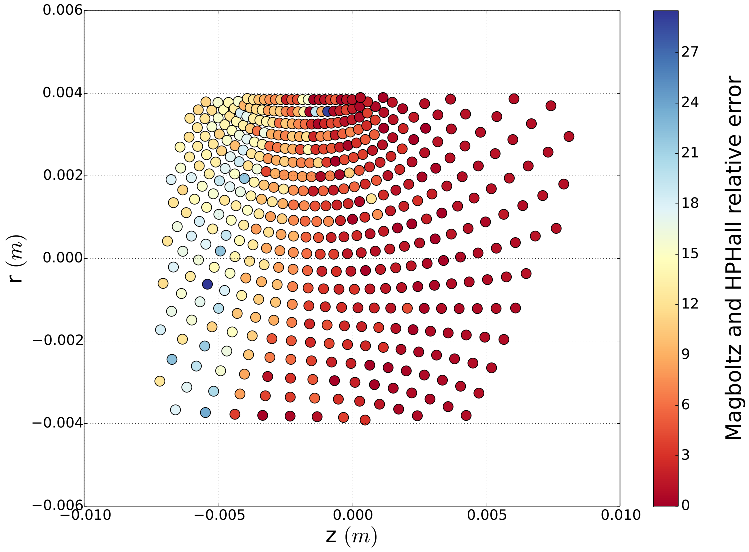


Figure 4: Ratio of HPHall to Magboltz perpendicular electron mobility (z=0 represent HET exitplane)

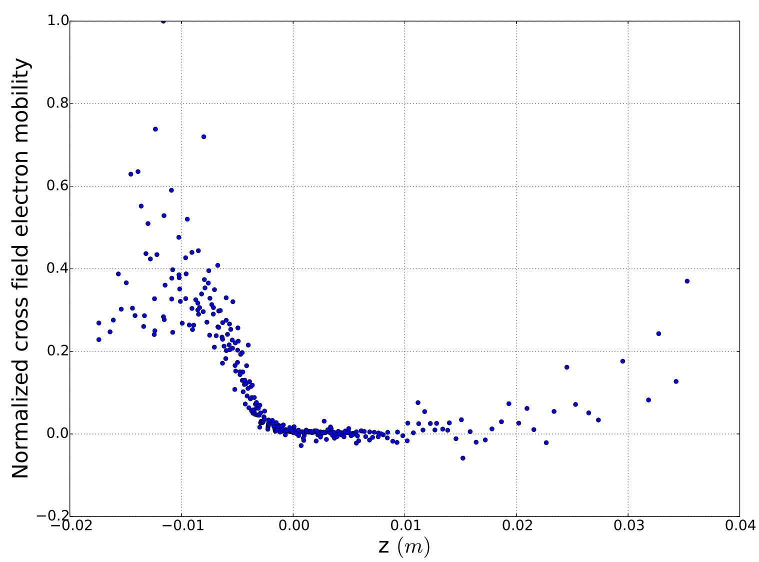


Figure 5: Normalized perpendicular electron mobility calculated by Magboltz (full dataset)

B. Mode B: 250V & 1.84A

The perpendicular electron mobility profiles for Mode B as calculated by HPHall and Magboltz are shown in Fig. 6. These data are normalized individually to the highest mobility shown in the field of view. The ratio between the two (HPHall divided by Magboltz) is shown in Fig. 7. Finally, the full dataset for the perpendicular electron mobility as calculated by Magboltz is shown in Fig. 8.

In this dataset, which represents a higher neutral flow than Mode A, there are some qualitative similarities between the overall Magboltz mobility in Fig. 8 and Fig. 1. In this case, instead of the greatest area of disagreement being in the near-anode region, it is instead in the classical mobility region of the thruster. Since this region is also inside the thruster exit plane, part of this discrepancy may be attributed to the additional electron-wall collision in HPHall; however, given the very narrow spatial extent of highest disagreement, there is likely some dependence on the Bohm transport contribution in this area. Regardless, it is clear that the curvature in the mobility profile is far steeper in HPHall than in Magboltz across the entire domain in Fig. 6 and this is strongly indicative that it is the Bohm transport contribution that is driving the HPHall solution.

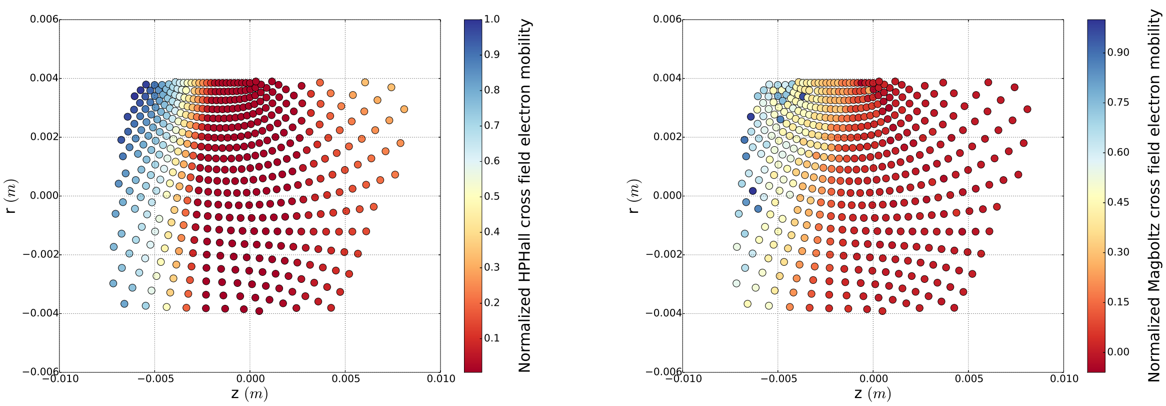


Figure 6: Relative perpendicular electron mobility calculated by HPHall (left) and Magboltz (right)

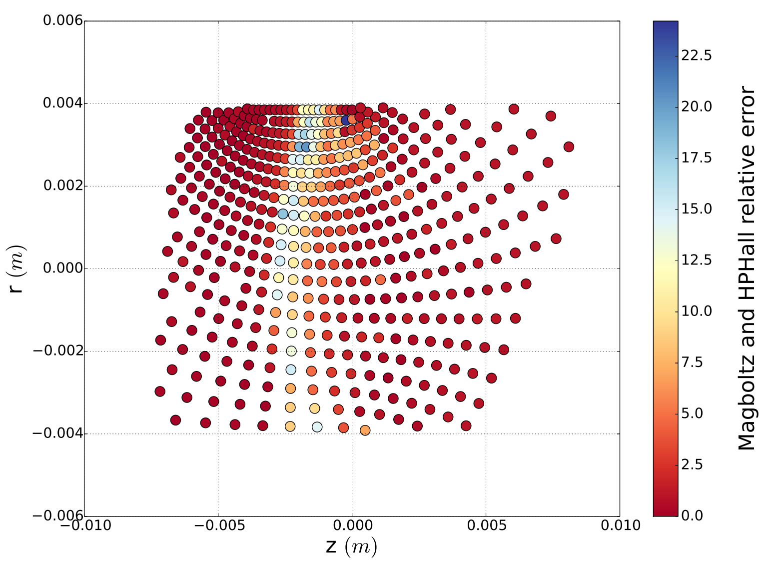


Figure 7: Ratio of HPHall to Magboltz perpendicular electron mobility (z=0 represent HET exitplane)

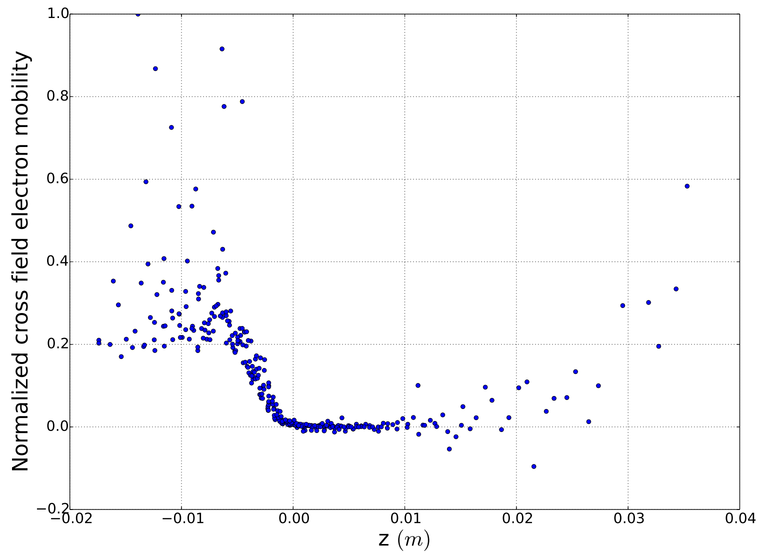
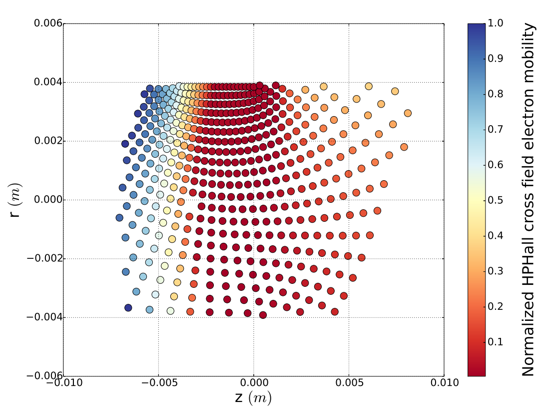


Figure 8: Normalized perpendicular electron mobility calculated by Magboltz (full dataset)

C. Mode C: 100V & 2.00A

The perpendicular electron mobility profiles for Mode C as calculated by HPHall and Magboltz are shown in Fig. 9. These data are normalized individually to the highest mobility shown in the field of view. The ratio between the two (HPHall divided by Magboltz) is shown in Fig. 10. Finally, the full dataset for the perpendicular electron mobility as calculated by Magboltz is shown in Fig. 11.

In this dataset, which has higher flow rate and lower magnetic field magnitude than Mode B, we again see the most disagreement in the region where classical mobility is most likely to be observed. This lower field magnitude results in a correspondingly larger contribution of the anomalous transport in the HPHall model ($\frac{1}{B^2}$ dependence), resulting in the relatively wide area of disagreement shown in Fig. 10.



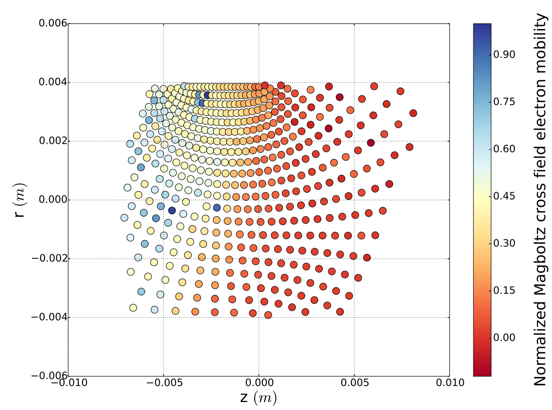


Figure 9: Relative perpendicular electron mobility calculated by HPHall (left) and Magboltz (right)

IV. Conclusion and future work

On the whole, Magboltz is found to notionally follow the expected classical mobility trends for regions within the channel and plume. Unfortunately, the mobility predicted by Magboltz differs greatly from the total mobility of HPHall. In some regions the difference is orders of magnitude. Therefore, while Magboltz does a significantly better job at predicting the mobility than a purely classical volumetric collision-based

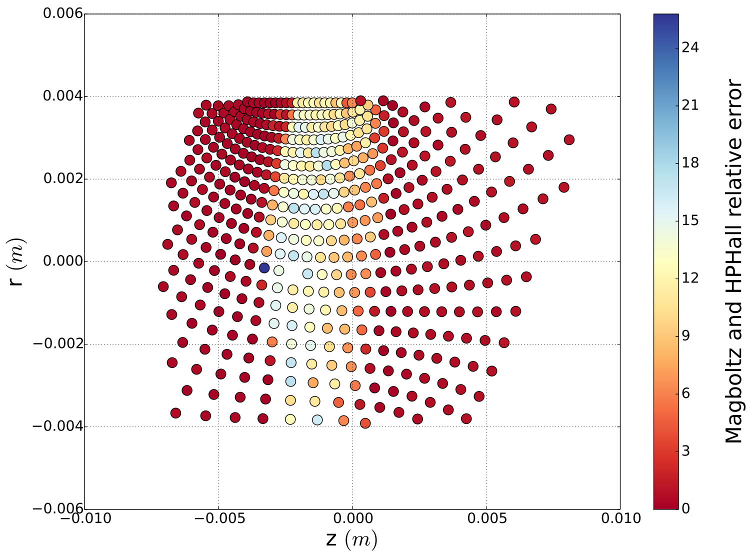


Figure 10: Ratio of HPHall to Magboltz perpendicular electron mobility (z=0 represent HET exitplane)

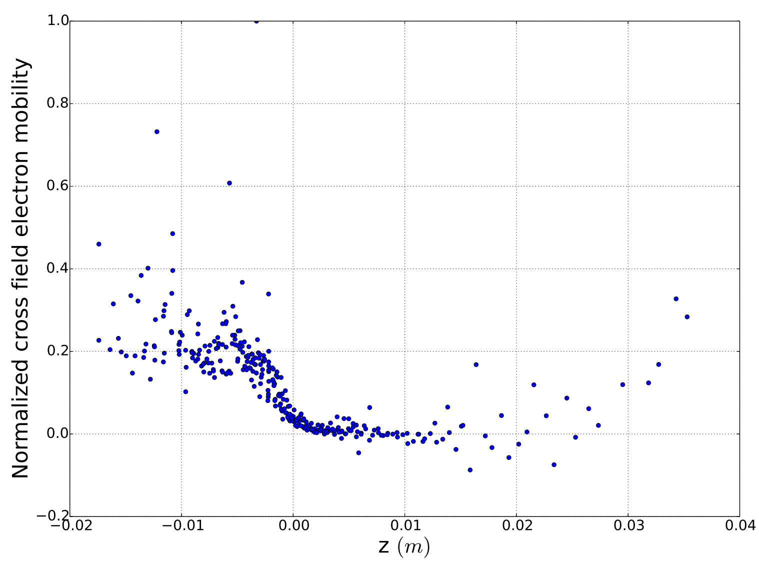


Figure 11: Normalized perpendicular electron mobility calculated by Magboltz (full dataset)

model, it alone cannot be expected to achieve the significant levels of mobility enhancement (represented by the anomalous collision models incorporated into HPHall) necessary for realistic HET simulation.

Nevertheless, as we move forward with improve HET simulations, the use of a tool like Magboltz to replace semi-empirical mobility models dependent of tuning parameters (such as the current generation of models in HPHall) would be a highly desirable means to access more physics-based mobility calculation. Unfortunately, obstacles to this remain, including the fact that the time to evaluate the diffusion tensor in Magboltz is currently measured in minutes instead of fractions of a second. To move forward and take advantage of the capabilities of Magboltz, we are considering the option of accelerating this process through the use of a tabulated database for mobility data recovered from Magboltz in the future.

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Boltzmann transport in hybrid-PIC HET modeling

06-10 Jul 2015

Jonathan Tran, Justin Koo, Robert Martin and Artan Qerushi

EP Modeling and Simulation group

AFRL/RQRS

Outline

- Motivation / description of numerical investigation
- Formulation of fluid electron mobility
- HPHall implementation of electron mobility
- Magboltz
  - Overview
  - Extracting mobility
- Comparison between HPHall and Magboltz
- Conclusions and future work

Motivation

- Common mechanisms for anomalous electron transport are turbulent field fluctuations and wall-collision effects
- Little explored mechanism in the HET literature is non-thermal equilibrium in the electron energy distribution
- Electron swarm codes such as Magboltz are readily accessible and allow for detailed calculation of transport coefficients
  – Assumes a balance between electrostatic force and collisional drag force in the presence of a magnetic field
- May reduce reliance on tunable parameters in evaluating the effective electron mobility for HET codes like HPHall

Formulation of effective electron mobility

From Generalized Ohm's law,

$$\vec{j_e} + \mu \vec{j_e} \times \vec{B} = \mu e n_e \vec{E} + \mu \nabla p$$

Making assumption that B=B_z and strict azimuthal symmetry,

$$j_x = \mu_\perp (e n_e E_x + \frac{\partial p}{\partial x})$$

where

$$\mu_\perp = \frac{\mu}{1+\mu^2 B^2} = \frac{e}{m\nu_e} \frac{1}{1+(\frac{eB}{m\nu_e})^2} = \frac{e}{m\nu_e} \frac{1}{1+\Omega_e^2}$$

and

$$\nu_e = \nu_{e,class} + \nu_{e,anom}$$

$$\nu_{e,class} = \nu_{e-ion} + \nu_{e-neutral}$$

$$\nu_{e,anom} = \nu_{wall} + \nu_{Bohm}$$

Requires semi-empirical models with tunable parameters to evaluate anomalous collision frequency

Effective mobility profiles

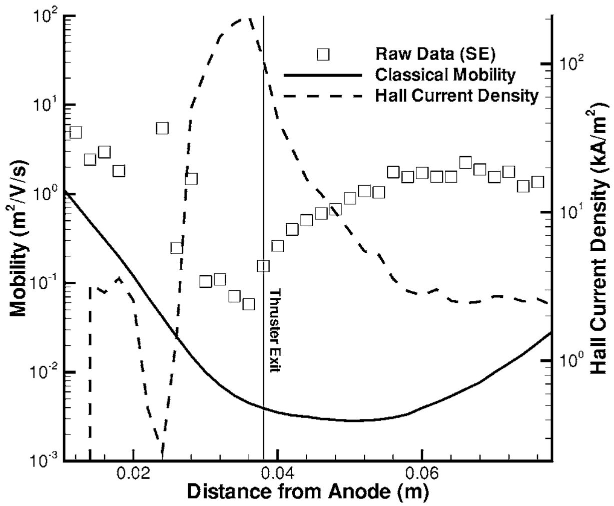
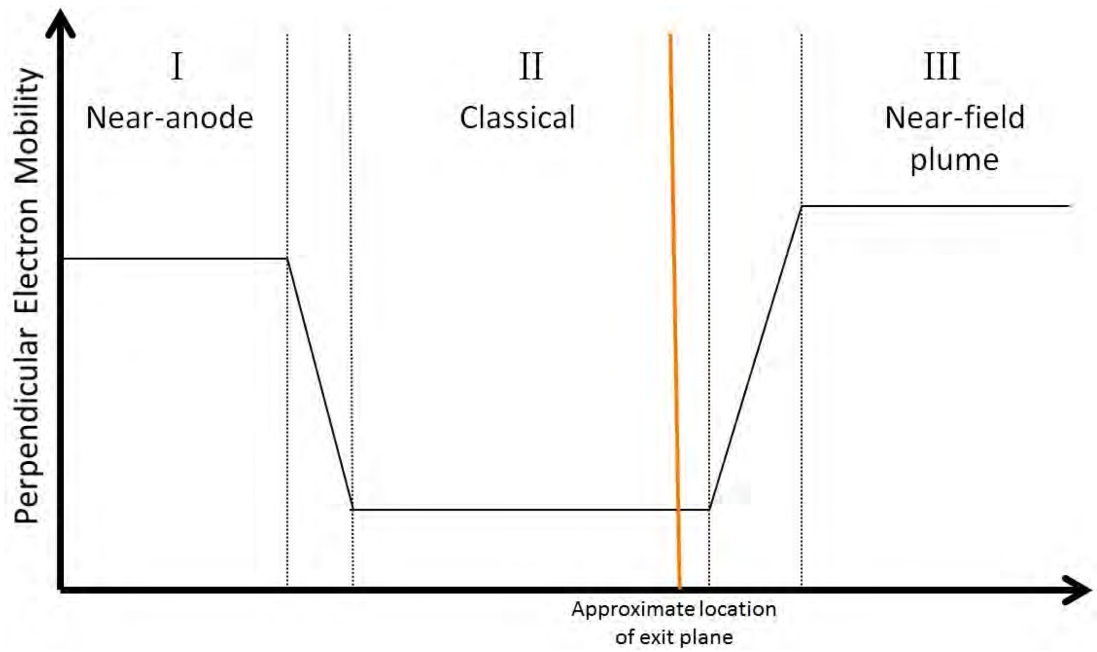


Figure from Koo, Justin W. and Boyd, Iain D., Modeling of anomalous electron mobility in Hall thrusters, Physics of Plasmas, 13, 033501 (2006)



Experience leads to observation that most effective electron mobility need aggressive anomalous correction in the near-field plume region

HPHall

JPL 3-region mobility model

- 2D axisymmetric hybrid PIC/MCC HET simulation code developed by J. Fife (MIT) and upgraded/managed by R. Hofer (NASA/JPL)
  - Particle ions (single/double) and neutrals
  - Electron temperature isothermal along magnetic field lines
  - Fixed background pressure
  - Fluid electrons
  - Fixed mdot, potential

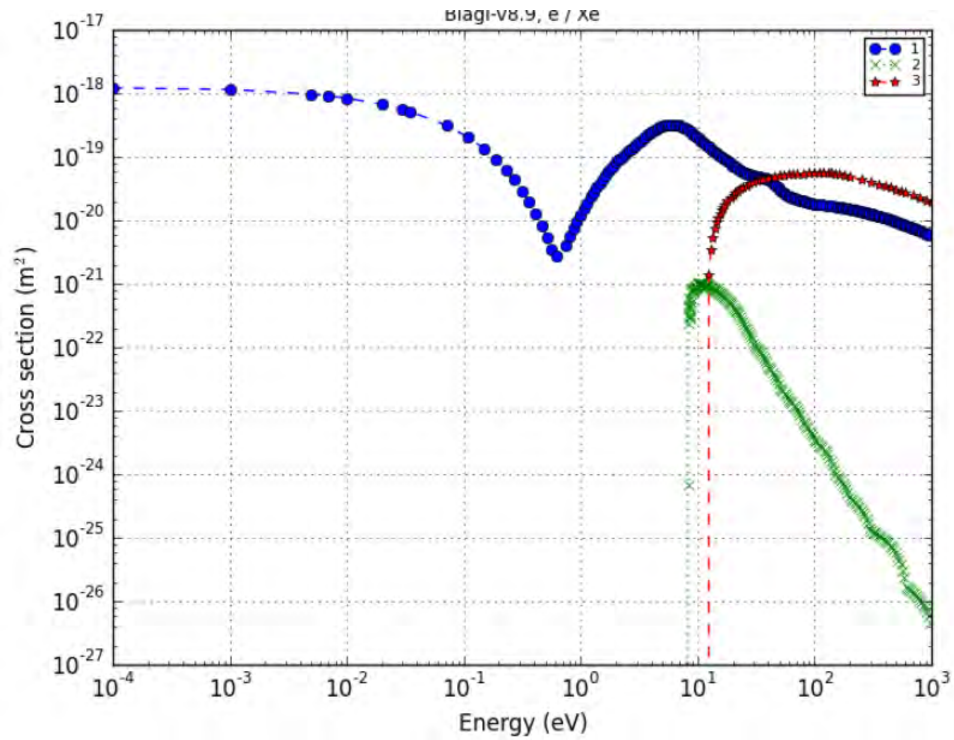
Case	Thrust (N)	Voltage (V)	Current (A)
Mode A	0.0137	250	0.80
Mode B	0.0265	250	1.84
Mode C	0.0141	100	2.00

Not tuned to experimental data – representative <1 kW HET

Figure from Hofer, R. R. et al, "Efficacy of Electron Mobility Models in Hybrid-PIC Hall Thruster Simulations," AIAA 2008-4924, 44th AIAA JPC Conference, Hartford, CT, 21-23 July 2008.

Magboltz Overview

- Developed by S. Biagi
- Performs analytical EM push of electrons with Monte Carlo elastic and inelastic collision mechanisms (E-field aligned with x-axis, B-field in x-z plane)
- Produces a 2nd rank symmetric diffusion tensor – diagonal only if E is perpendicular to B
- Uses 52 e-Xe collision cross sections from `www.lxcat.net`
- Runs hundreds of thousands of particle flight (~1 minute) to produce a diffusion tensor



Extracting Mobility

- Diffusion tensor is calculated by evaluating

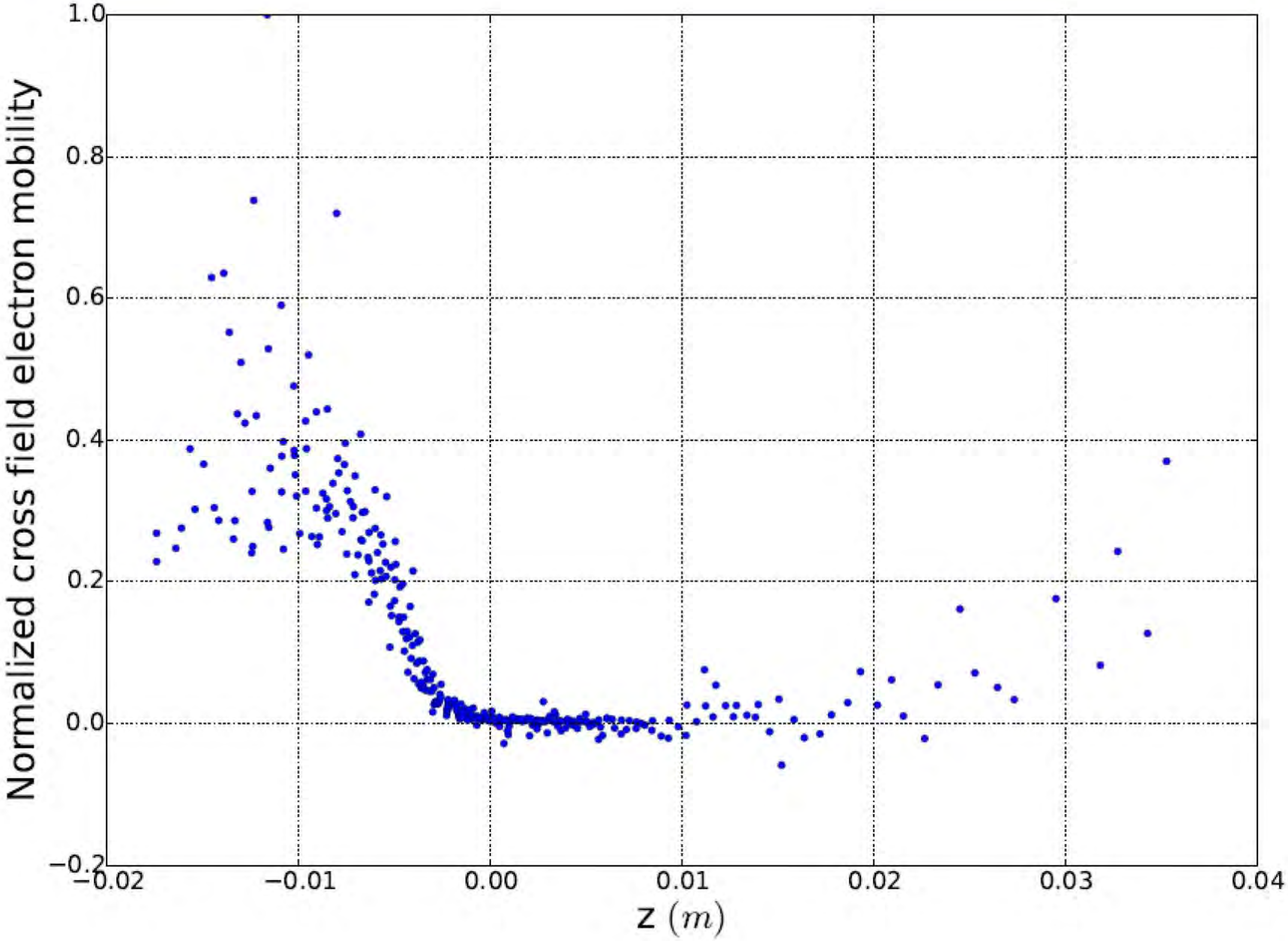
$$D_{ij} = \frac{1}{2N}\sum\left[\frac{1}{dt}(q_i - v_i dt)(q_j - v_j dt)\right]$$

- Mobility tensor is 2nd rank antisymmetric tensor
- Focus on extracting cross field (i.e. smallest) component of diffusion tensor
  - Diagonalize D_{ij} or calculate eigenvalues
  - Smallest eigenvalue is perpendicular component of diffusion tensor
- Use Einstein relation to recover perpendicular electron mobility coefficient

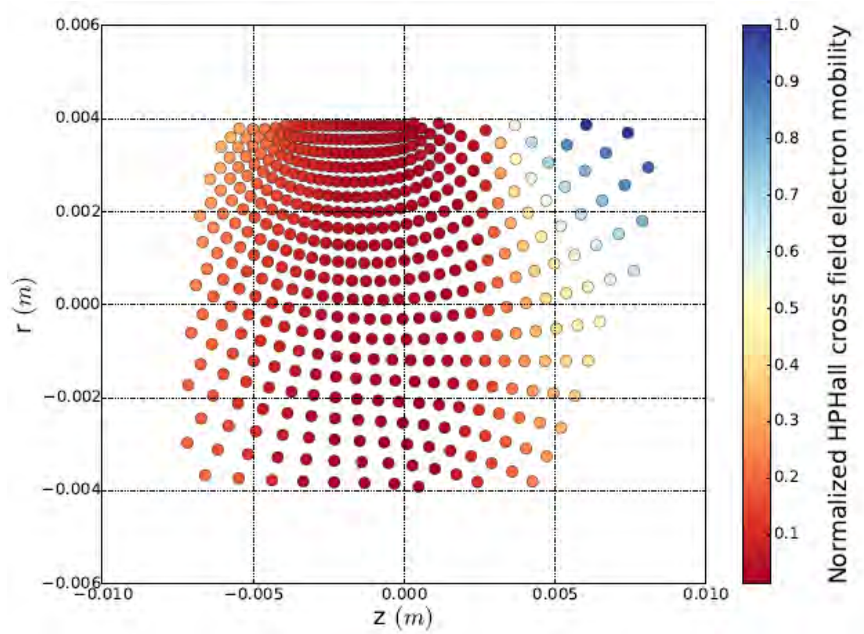
$$\frac{D_\perp}{\mu_\perp} = \frac{k_B T_e}{e}$$

Mode A

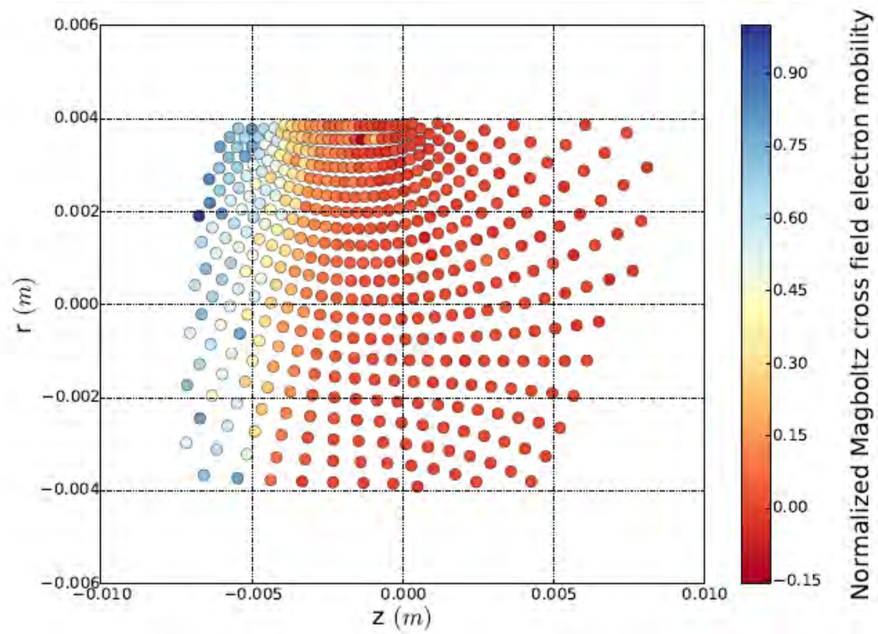
250 V & 0.80 A



Mode A
250 V & 0.80 A

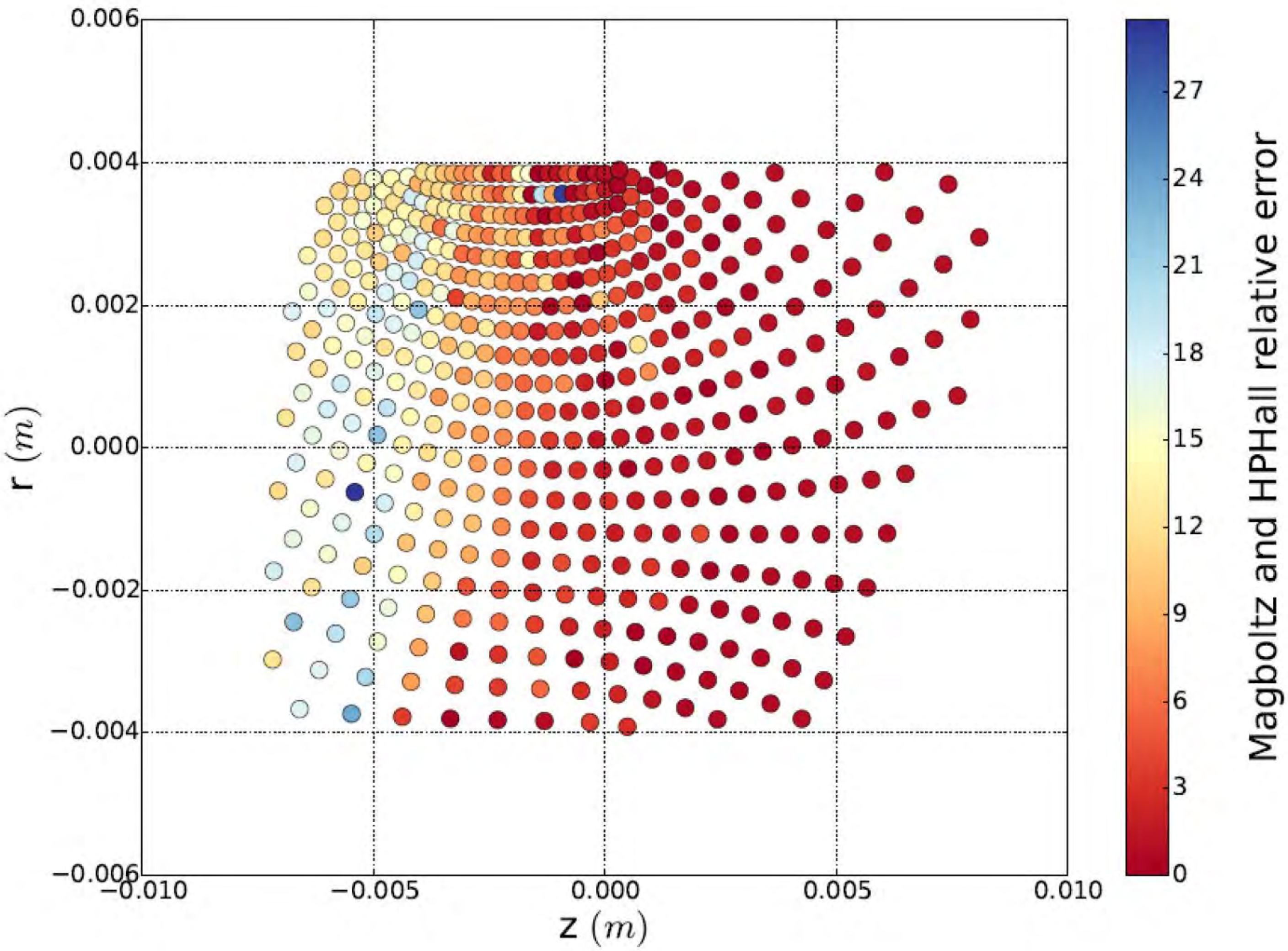


HPHall

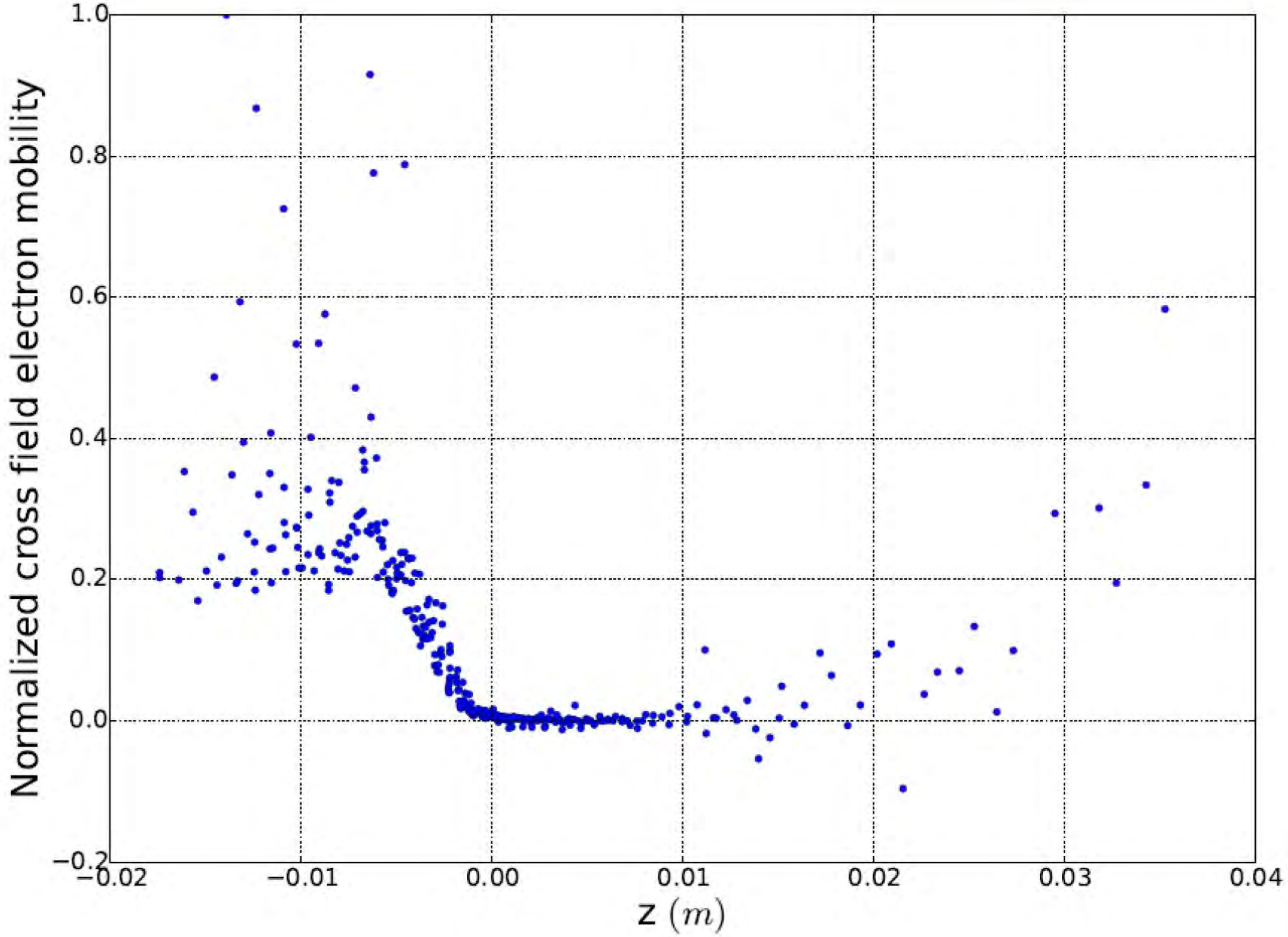


Magboltz

Mode A
250 V & 0.80 A

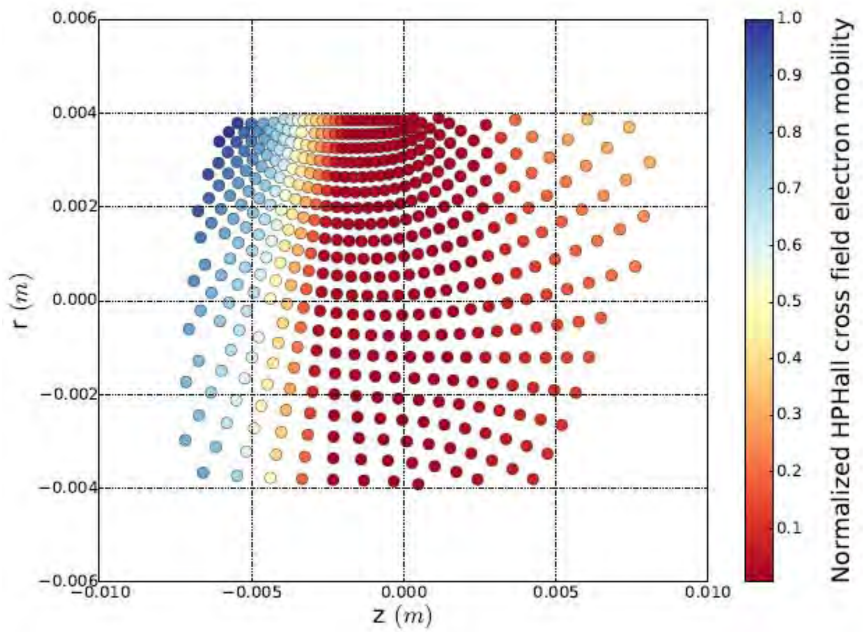


Mode B
250 V & 1.84 A



Mode B

250 V & 1.84 A



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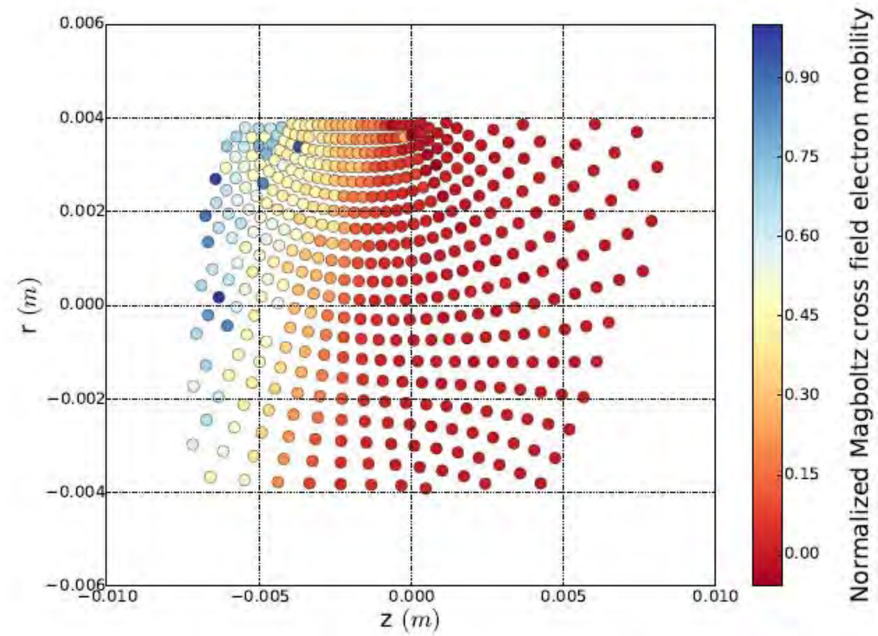
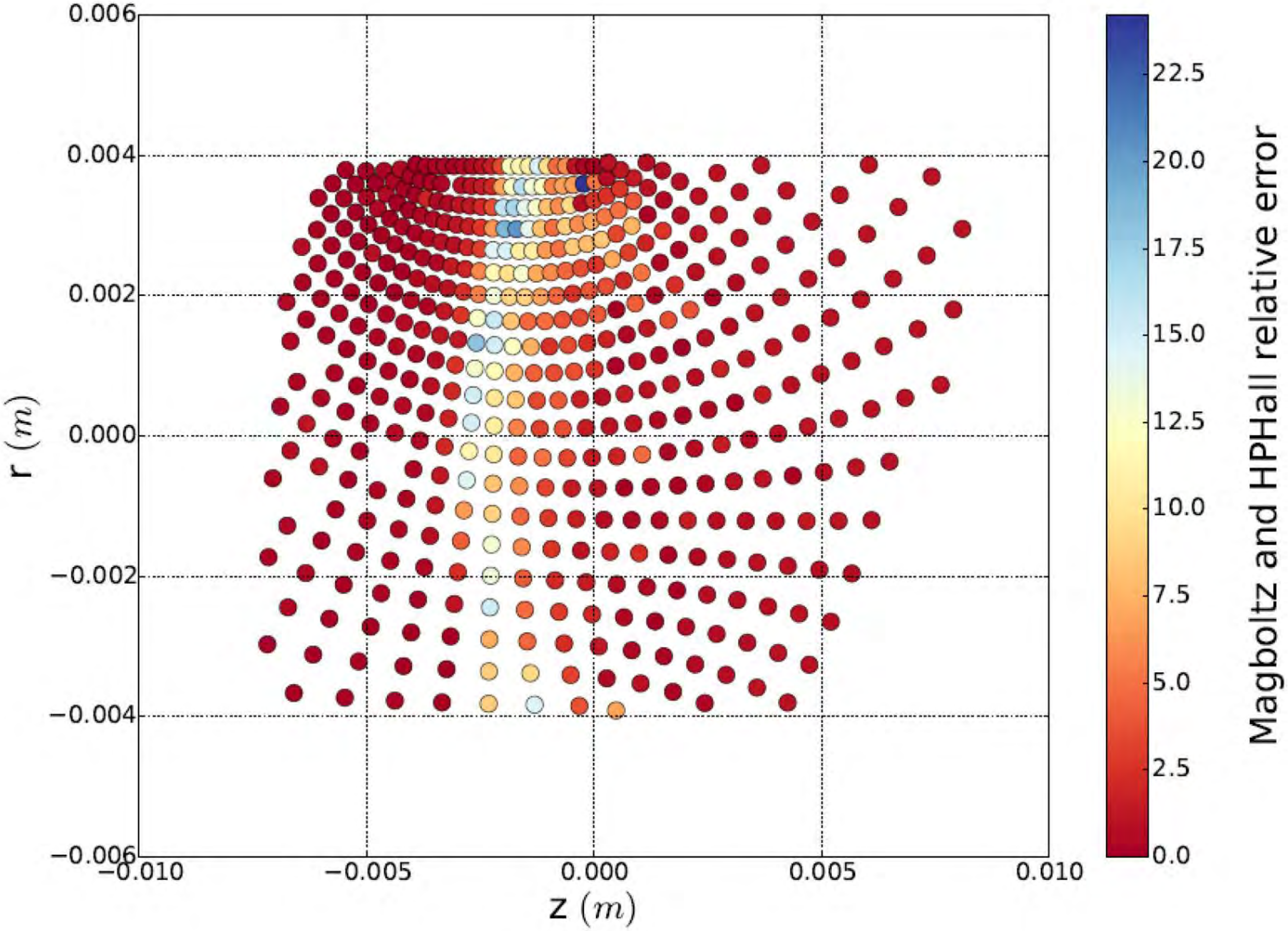
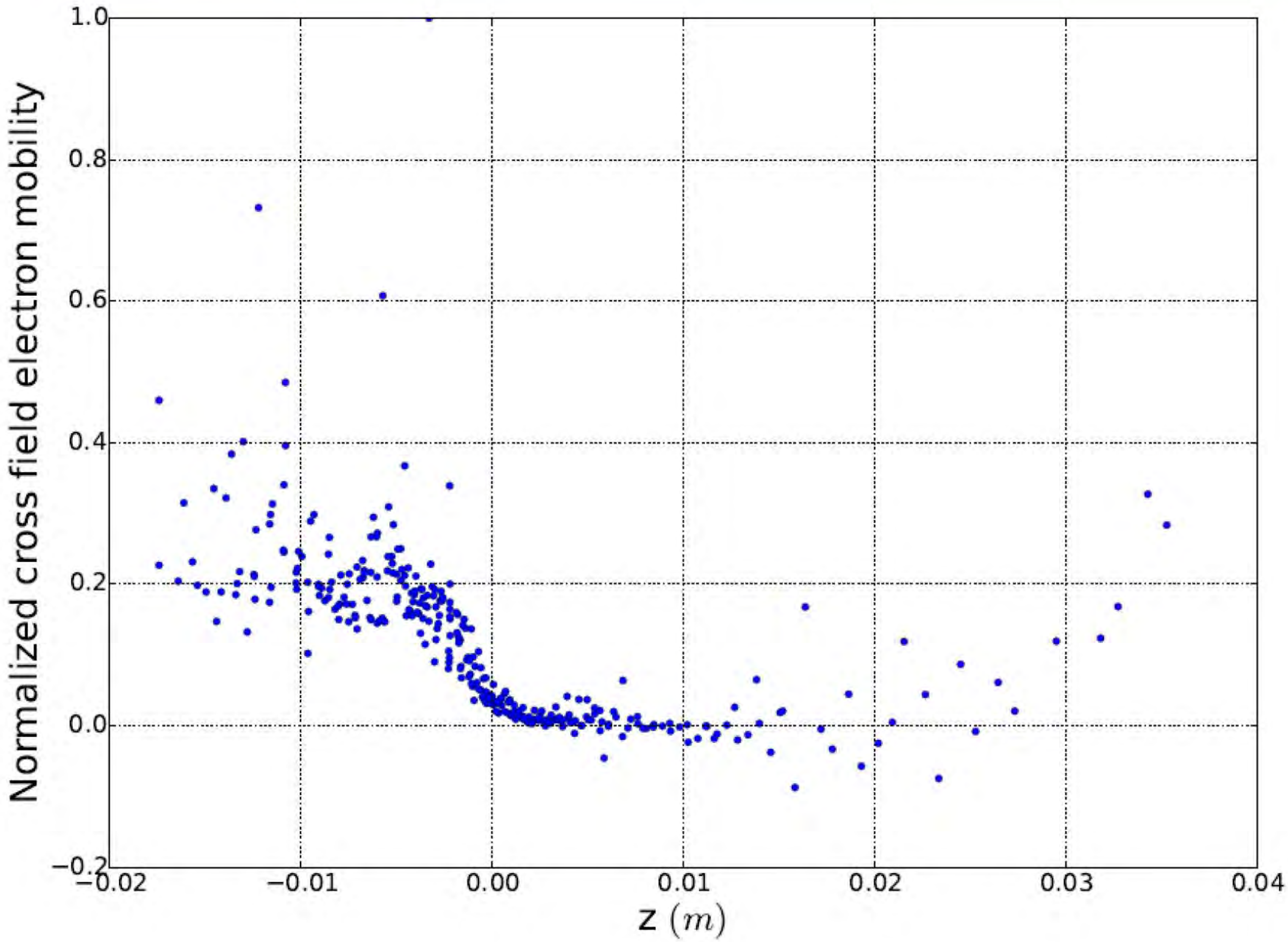


Magboltz

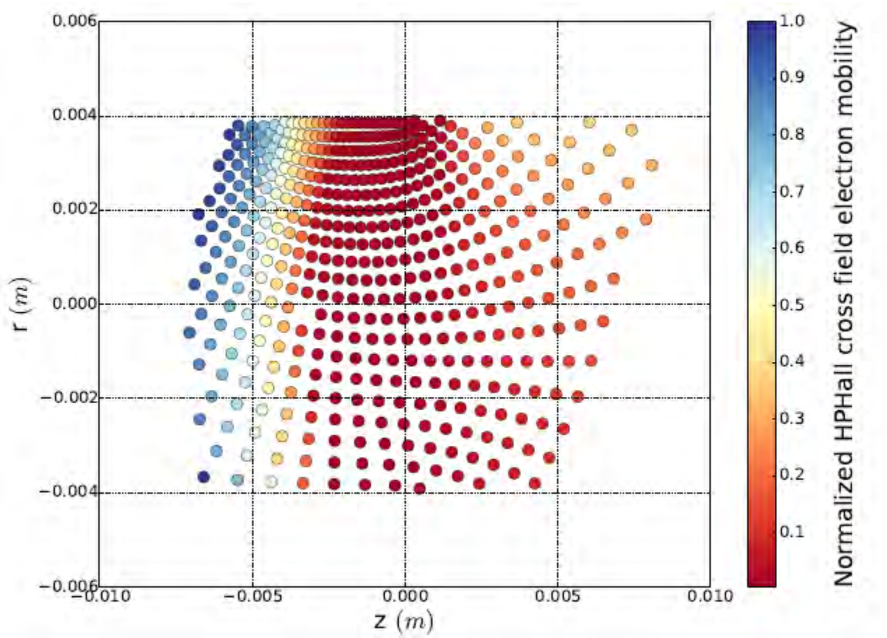
Mode B
250 V & 1.84 A



Mode C
100 V & 2.00 A



Mode C
100 V & 2.00 A



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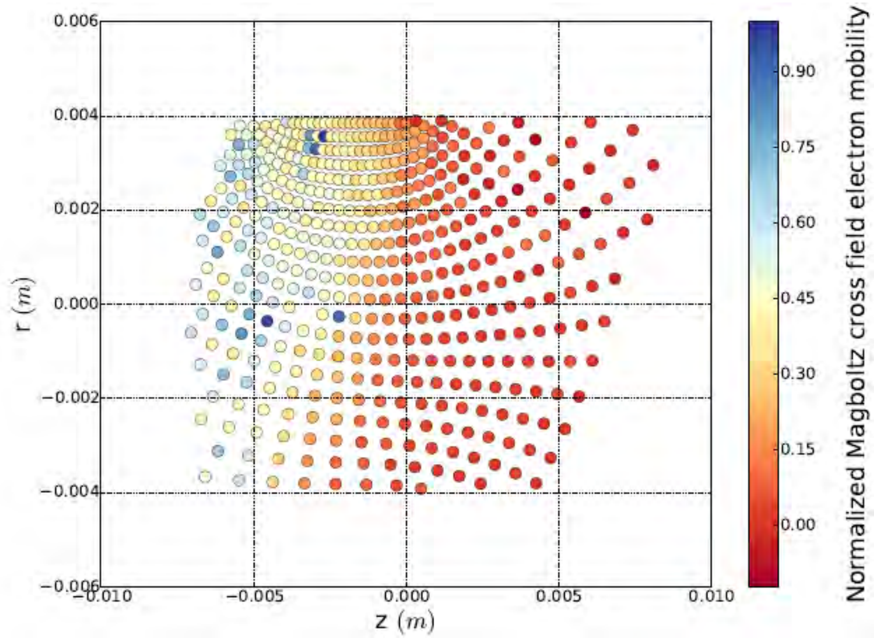
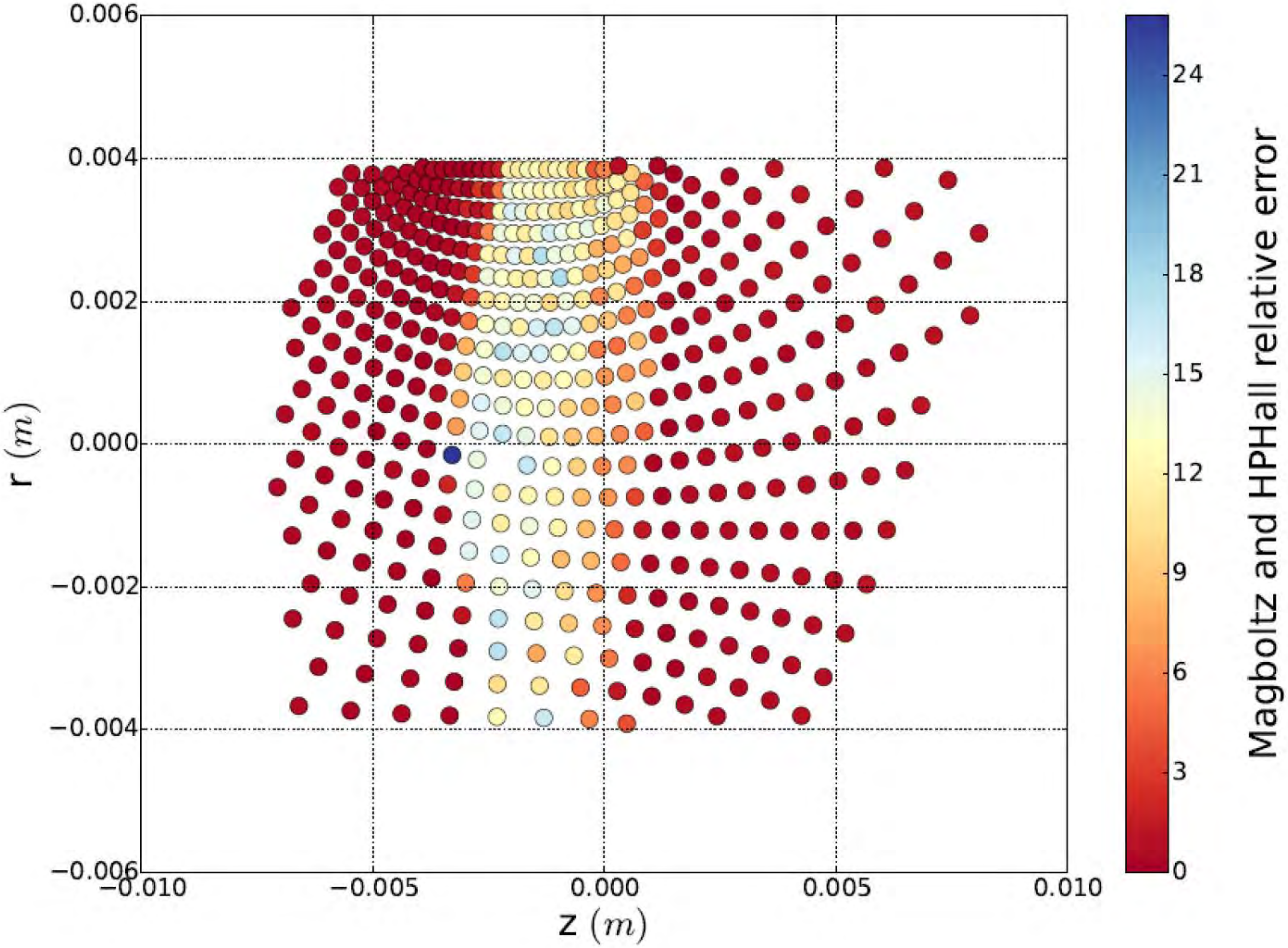


Magboltz

Mode C
100 V & 2.00 A



Summary and Future Work

- Magboltz generally produces a higher mobility than purely classical volumetric collision-based methods
- Unfortunately, does not offer sufficient additional transport to reach level required for reasonable HET simulation
- Too slow to be directly incorporated into a time-dependent HET model
  - Investigating parametrizing the output to build a faster table lookup capability